



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 10, 2021 – 07:18 PM EDT

PDB ID : 3DBL  
Title : Structural Dissection of a Gating Mechanism Preventing Misactivation of Ubiquitin by NEDD8's E1 (APPBP1-UBA3Arg190wt-NEDD8Ala72Gln)  
Authors : Souphron, J.; Schulman, B.A.  
Deposited on : 2008-06-01  
Resolution : 2.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

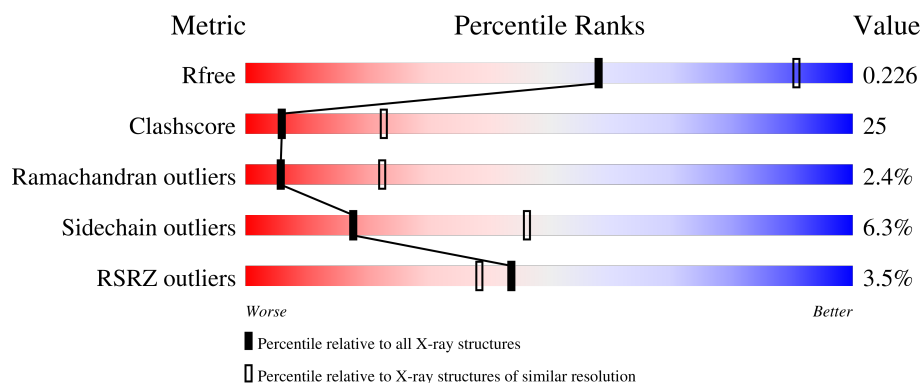
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	531	<div> <div>2%</div> <div> <div></div> <div>60%</div> <div>35%</div> <div>..</div> </div> </div>
1	C	531	<div> <div>%</div> <div> <div></div> <div>60%</div> <div>34%</div> <div>..</div> </div> </div>
1	E	531	<div> <div>2%</div> <div> <div></div> <div>60%</div> <div>34%</div> <div>..</div> </div> </div>
1	G	531	<div> <div>3%</div> <div> <div></div> <div>59%</div> <div>35%</div> <div>..</div> </div> </div>
2	B	434	<div> <div>4%</div> <div> <div></div> <div>52%</div> <div>41%</div> <div>5% .</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	D	434	<div><div></div><div>4%</div><div>57%</div><div>38%</div><div>5%</div></div>
2	F	434	<div><div></div><div>6%</div><div>52%</div><div>40%</div><div>6%</div><div>••</div></div>
2	H	434	<div><div></div><div>6%</div><div>49%</div><div>44%</div><div>6%</div><div>•</div></div>
3	I	88	<div><div></div><div>60%</div><div>34%</div><div>•</div><div>•</div></div>
3	J	88	<div><div></div><div>3%</div><div>48%</div><div>33%</div><div>6%</div><div>14%</div></div>
3	K	88	<div><div></div><div>%</div><div>41%</div><div>40%</div><div>5%</div><div>•</div><div>14%</div></div>
3	L	88	<div><div></div><div>6%</div><div>31%</div><div>51%</div><div>5%</div><div>14%</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 32577 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NEDD8-activating enzyme E1 regulatory subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	522	Total	C	N	O	S	0	0	0
			4138	2621	704	797	16			
1	C	520	Total	C	N	O	S	0	0	0
			4125	2612	702	795	16			
1	E	521	Total	C	N	O	S	0	0	0
			4119	2609	703	792	15			
1	G	518	Total	C	N	O	S	0	0	0
			4113	2605	700	793	15			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q13564
A	0	SER	-	expression tag	UNP Q13564
A	?	-	ASN	deletion	UNP Q13564
A	?	-	GLU	deletion	UNP Q13564
A	?	-	ASN	deletion	UNP Q13564
A	?	-	GLY	deletion	UNP Q13564
A	?	-	ALA	deletion	UNP Q13564
C	-1	GLY	-	expression tag	UNP Q13564
C	0	SER	-	expression tag	UNP Q13564
C	?	-	ASN	deletion	UNP Q13564
C	?	-	GLU	deletion	UNP Q13564
C	?	-	ASN	deletion	UNP Q13564
C	?	-	GLY	deletion	UNP Q13564
C	?	-	ALA	deletion	UNP Q13564
E	-1	GLY	-	expression tag	UNP Q13564
E	0	SER	-	expression tag	UNP Q13564
E	?	-	ASN	deletion	UNP Q13564
E	?	-	GLU	deletion	UNP Q13564
E	?	-	ASN	deletion	UNP Q13564
E	?	-	GLY	deletion	UNP Q13564
E	?	-	ALA	deletion	UNP Q13564

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-1	GLY	-	expression tag	UNP Q13564
G	0	SER	-	expression tag	UNP Q13564
G	?	-	ASN	deletion	UNP Q13564
G	?	-	GLU	deletion	UNP Q13564
G	?	-	ASN	deletion	UNP Q13564
G	?	-	GLY	deletion	UNP Q13564
G	?	-	ALA	deletion	UNP Q13564

- Molecule 2 is a protein called NEDD8-activating enzyme E1 catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	432	Total	C	N	O	S	0	0	0
			3404	2175	577	635	17			
2	D	432	Total	C	N	O	S	0	0	0
			3408	2178	578	635	17			
2	F	431	Total	C	N	O	S	0	0	0
			3397	2172	576	632	17			
2	H	431	Total	C	N	O	S	0	0	0
			3389	2165	575	632	17			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	9	MET	-	expression tag	UNP Q8TBC4
B	10	LYS	-	expression tag	UNP Q8TBC4
B	11	LEU	-	expression tag	UNP Q8TBC4
B	216	ALA	CYS	engineered mutation	UNP Q8TBC4
D	9	MET	-	expression tag	UNP Q8TBC4
D	10	LYS	-	expression tag	UNP Q8TBC4
D	11	LEU	-	expression tag	UNP Q8TBC4
D	216	ALA	CYS	engineered mutation	UNP Q8TBC4
F	9	MET	-	expression tag	UNP Q8TBC4
F	10	LYS	-	expression tag	UNP Q8TBC4
F	11	LEU	-	expression tag	UNP Q8TBC4
F	216	ALA	CYS	engineered mutation	UNP Q8TBC4
H	9	MET	-	expression tag	UNP Q8TBC4
H	10	LYS	-	expression tag	UNP Q8TBC4
H	11	LEU	-	expression tag	UNP Q8TBC4
H	216	ALA	CYS	engineered mutation	UNP Q8TBC4

- Molecule 3 is a protein called NEDD8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	86	Total 668	C 415	N 121	O 130	S 2	0	0	0
3	J	76	Total 604	C 380	N 105	O 117	S 2	0	0	0
3	K	76	Total 604	C 380	N 105	O 117	S 2	0	0	0
3	L	76	Total 604	C 380	N 105	O 117	S 2	0	0	0

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	89	GLY	-	expression tag	UNP Q15843
I	90	SER	-	expression tag	UNP Q15843
I	91	ARG	-	expression tag	UNP Q15843
I	92	ARG	-	expression tag	UNP Q15843
I	93	ALA	-	expression tag	UNP Q15843
I	94	SER	-	expression tag	UNP Q15843
I	95	VAL	-	expression tag	UNP Q15843
I	96	GLY	-	expression tag	UNP Q15843
I	97	SER	-	expression tag	UNP Q15843
I	98	GLY	-	expression tag	UNP Q15843
I	99	GLY	-	expression tag	UNP Q15843
I	100	SER	-	expression tag	UNP Q15843
I	172	GLN	ALA	engineered mutation	UNP Q15843
J	89	GLY	-	expression tag	UNP Q15843
J	90	SER	-	expression tag	UNP Q15843
J	91	ARG	-	expression tag	UNP Q15843
J	92	ARG	-	expression tag	UNP Q15843
J	93	ALA	-	expression tag	UNP Q15843
J	94	SER	-	expression tag	UNP Q15843
J	95	VAL	-	expression tag	UNP Q15843
J	96	GLY	-	expression tag	UNP Q15843
J	97	SER	-	expression tag	UNP Q15843
J	98	GLY	-	expression tag	UNP Q15843
J	99	GLY	-	expression tag	UNP Q15843
J	100	SER	-	expression tag	UNP Q15843
J	172	GLN	ALA	engineered mutation	UNP Q15843
K	89	GLY	-	expression tag	UNP Q15843
K	90	SER	-	expression tag	UNP Q15843
K	91	ARG	-	expression tag	UNP Q15843
K	92	ARG	-	expression tag	UNP Q15843
K	93	ALA	-	expression tag	UNP Q15843

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Chain	Residue	Modelled	Actual	Comment	Reference
K	94	SER	-	expression tag	UNP Q15843
K	95	VAL	-	expression tag	UNP Q15843
K	96	GLY	-	expression tag	UNP Q15843
K	97	SER	-	expression tag	UNP Q15843
K	98	GLY	-	expression tag	UNP Q15843
K	99	GLY	-	expression tag	UNP Q15843
K	100	SER	-	expression tag	UNP Q15843
K	172	GLN	ALA	engineered mutation	UNP Q15843
L	89	GLY	-	expression tag	UNP Q15843
L	90	SER	-	expression tag	UNP Q15843
L	91	ARG	-	expression tag	UNP Q15843
L	92	ARG	-	expression tag	UNP Q15843
L	93	ALA	-	expression tag	UNP Q15843
L	94	SER	-	expression tag	UNP Q15843
L	95	VAL	-	expression tag	UNP Q15843
L	96	GLY	-	expression tag	UNP Q15843
L	97	SER	-	expression tag	UNP Q15843
L	98	GLY	-	expression tag	UNP Q15843
L	99	GLY	-	expression tag	UNP Q15843
L	100	SER	-	expression tag	UNP Q15843
L	172	GLN	ALA	engineered mutation	UNP Q15843

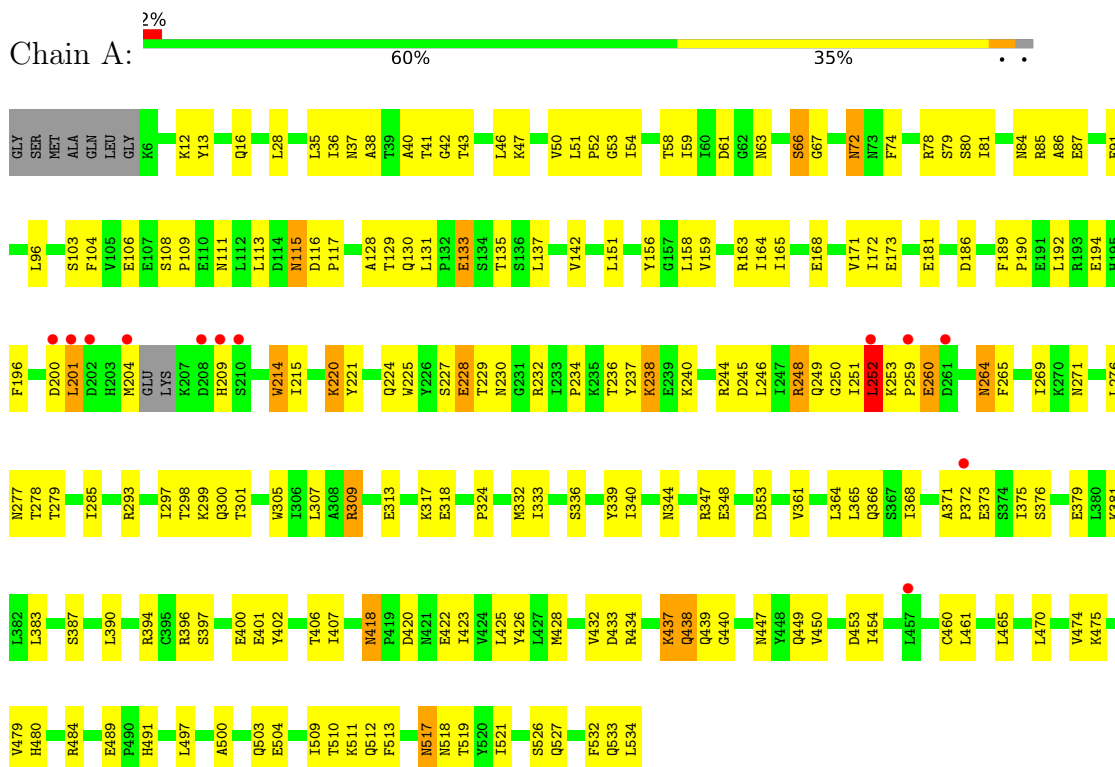
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Zn 1 1	0	0
4	D	1	Total Zn 1 1	0	0
4	F	1	Total Zn 1 1	0	0
4	H	1	Total Zn 1 1	0	0

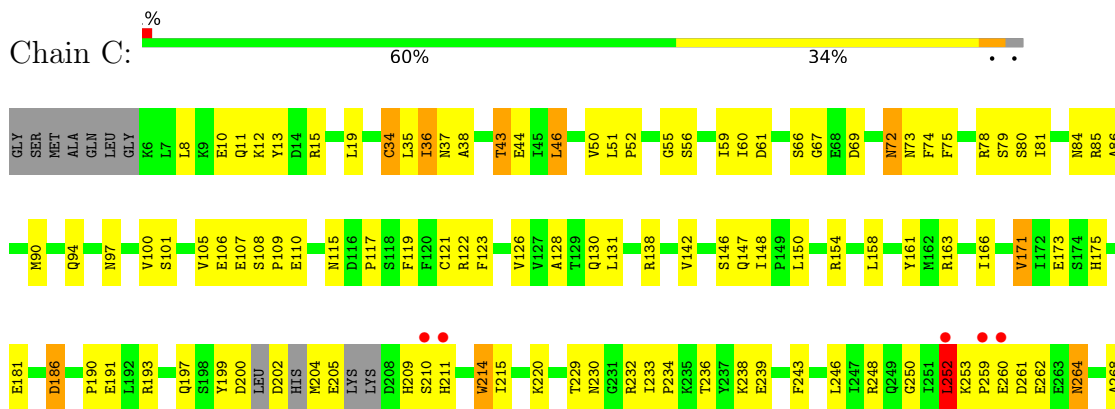
### 3 Residue-property plots [i](#)

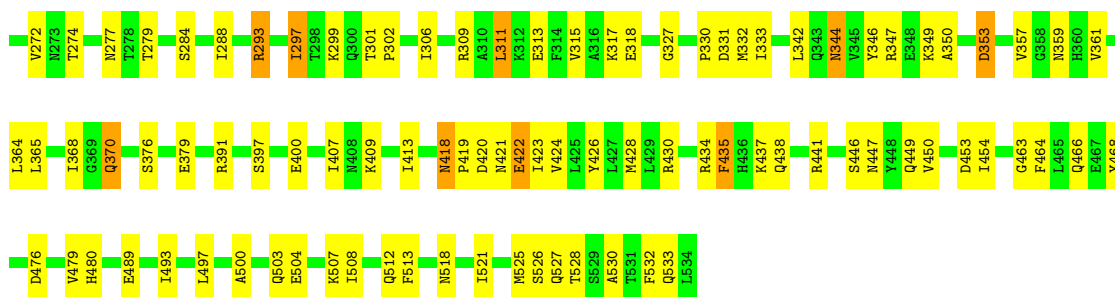
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: NEDD8-activating enzyme E1 regulatory subunit

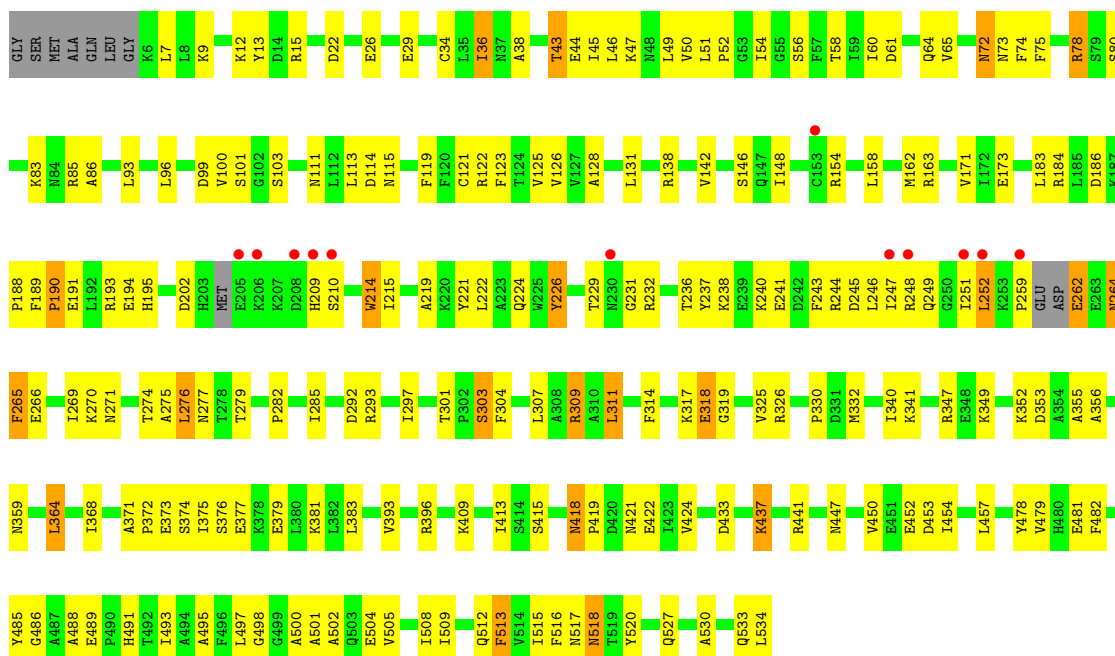


- Molecule 1: NEDD8-activating enzyme E1 regulatory subunit

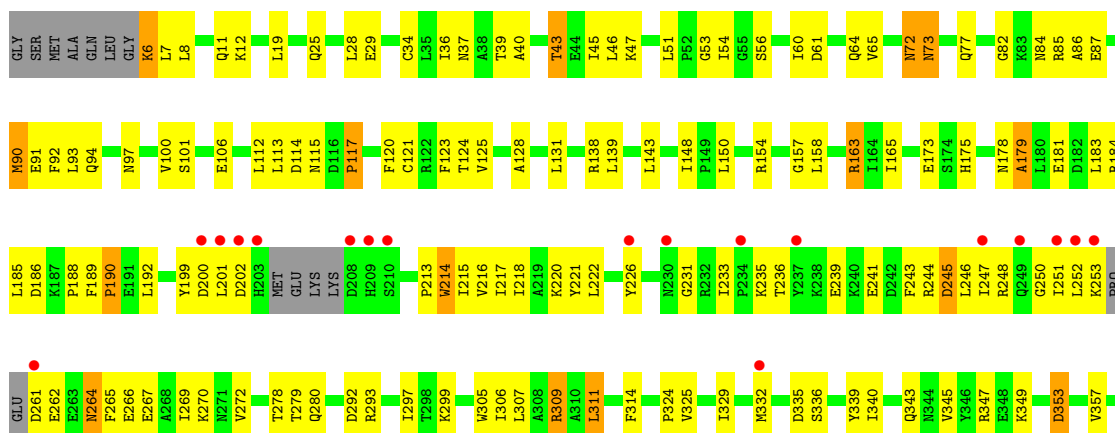


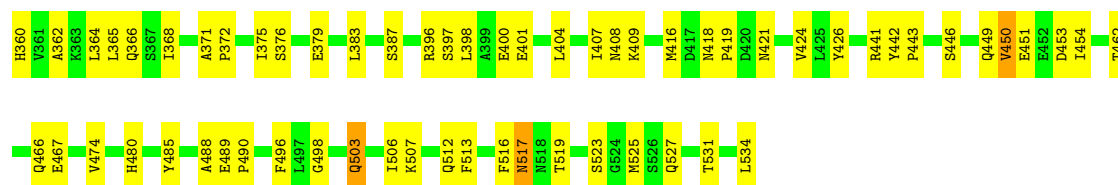


• Molecule 1: NEDD8-activating enzyme E1 regulatory subunit

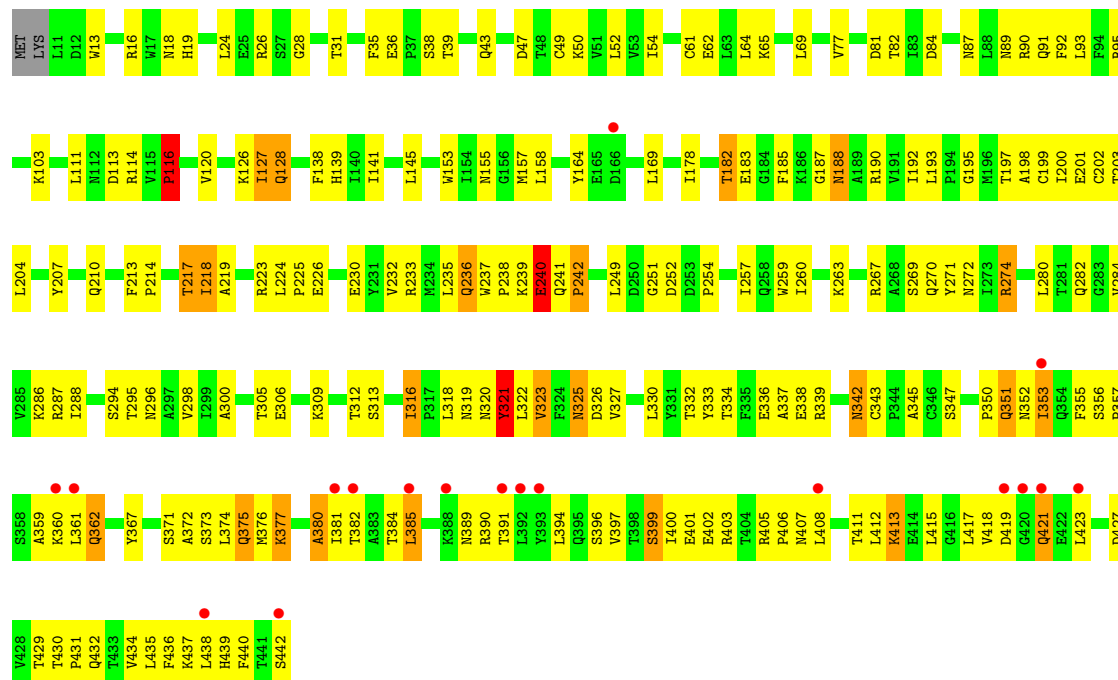


• Molecule 1: NEDD8-activating enzyme E1 regulatory subunit

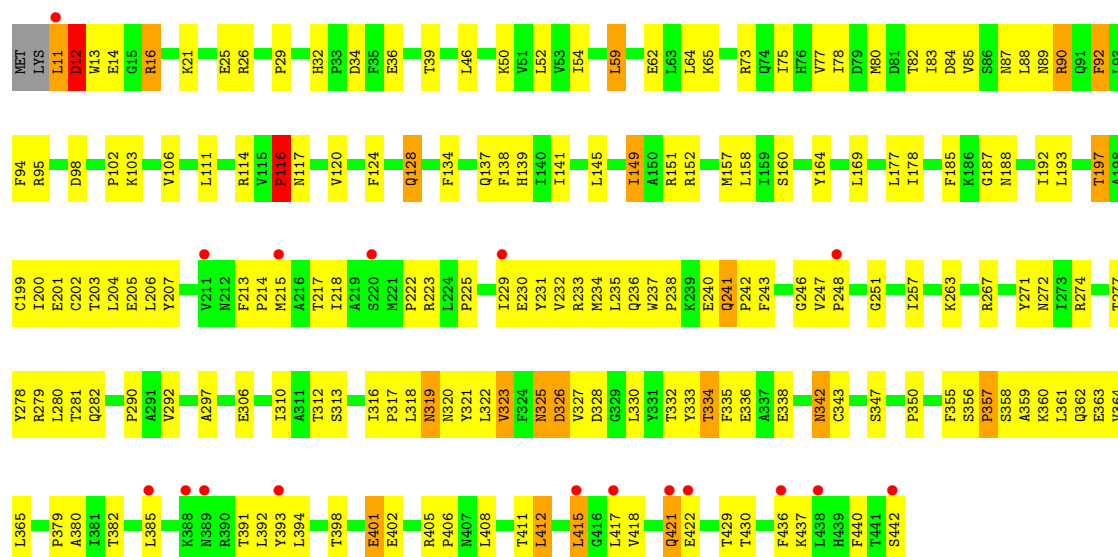




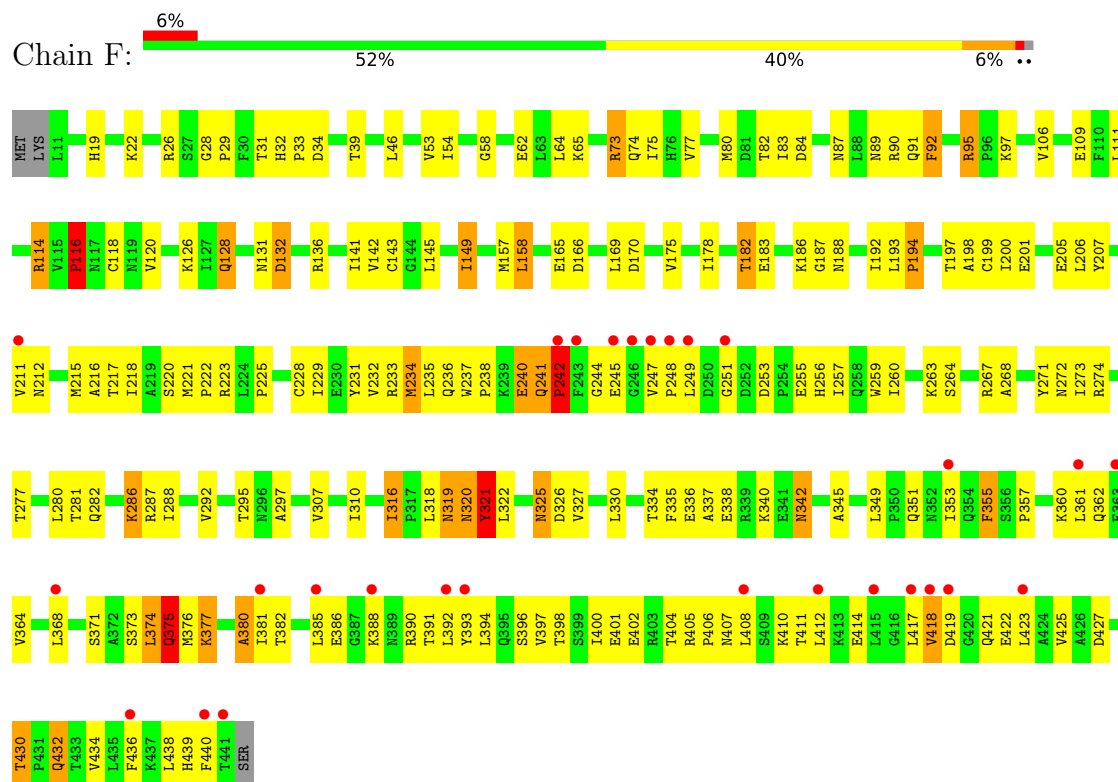
• Molecule 2: NEDD8-activating enzyme E1 catalytic subunit



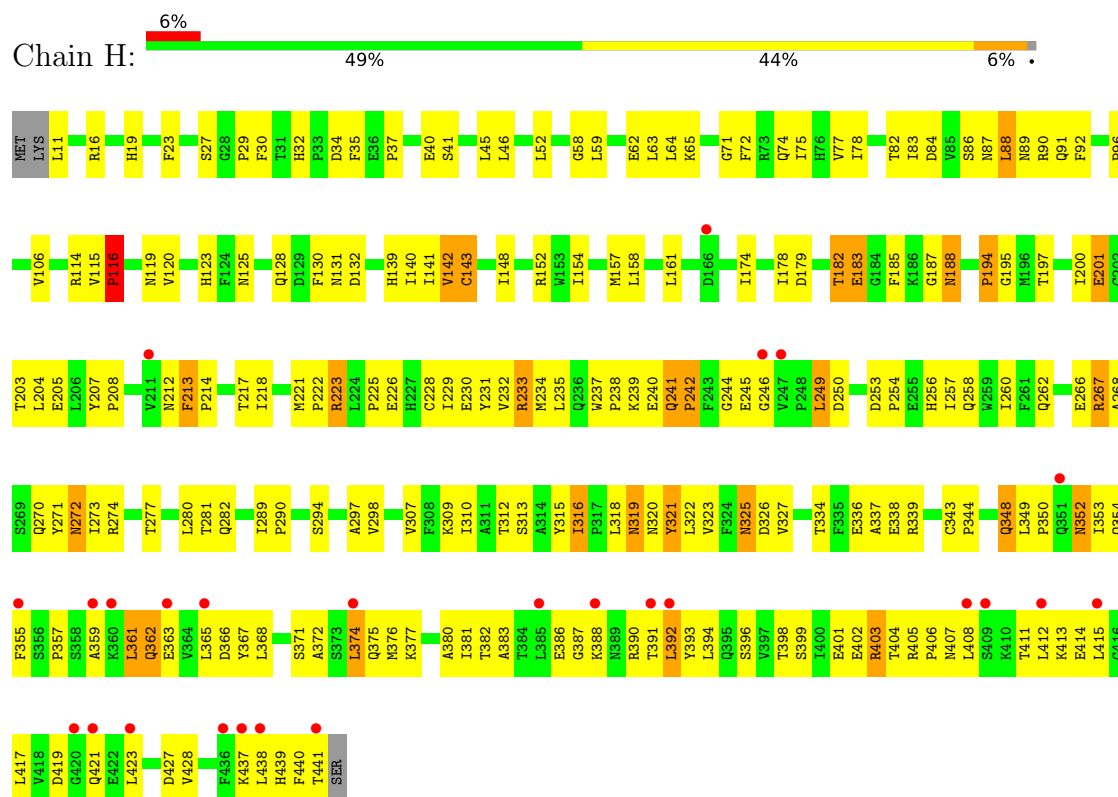
• Molecule 2: NEDD8-activating enzyme E1 catalytic subunit



- Molecule 2: NEDD8-activating enzyme E1 catalytic subunit



- Molecule 2: NEDD8-activating enzyme E1 catalytic subunit



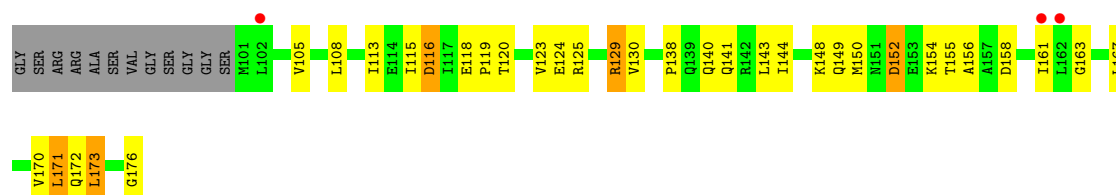
- Molecule 3: NEDD8

Chain I:  60% 34% . .



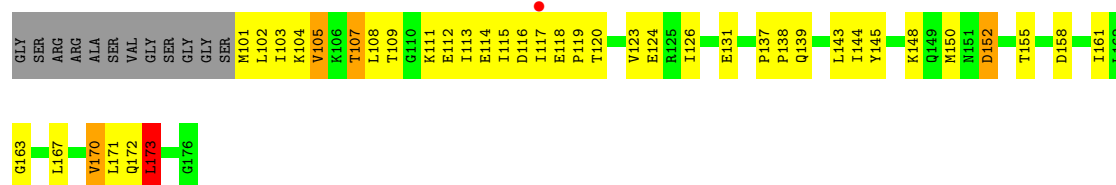
• Molecule 3: NEDD8

Chain J:  3% 48% 33% 6% 14%



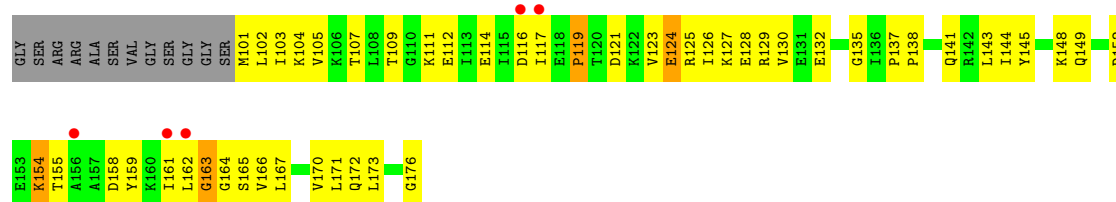
• Molecule 3: NEDD8

Chain K:  % 41% 40% 5% 14%



• Molecule 3: NEDD8

Chain L:  6% 31% 51% 5% 14%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	136.12Å 198.95Å 210.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.90 48.99 – 2.91	Depositor EDS
% Data completeness (in resolution range)	92.2 (50.00-2.90) 92.7 (48.99-2.91)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.07 (at 2.91Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.225 , 0.274 0.227 , 0.226	Depositor DCC
$R_{free}$ test set	5854 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	61.0	Xtriage
Anisotropy	0.487	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 46.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	32577	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.15% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.43	0/4218	0.67	0/5706
1	C	0.41	0/4203	0.62	0/5682
1	E	0.45	0/4198	0.66	0/5678
1	G	0.43	0/4191	0.64	0/5668
2	B	0.47	1/3482 (0.0%)	0.71	2/4738 (0.0%)
2	D	0.44	0/3486	0.67	1/4742 (0.0%)
2	F	0.51	1/3475 (0.0%)	0.75	3/4730 (0.1%)
2	H	0.46	0/3467	0.71	2/4720 (0.0%)
3	I	0.44	0/673	0.68	0/897
3	J	0.42	0/609	0.70	0/813
3	K	0.48	0/609	0.75	1/813 (0.1%)
3	L	0.38	0/609	0.67	0/813
All	All	0.45	2/33220 (0.0%)	0.68	9/45000 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	380	ALA	CA-CB	-9.09	1.33	1.52
2	B	380	ALA	CA-CB	-5.91	1.40	1.52

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	165	GLU	N-CA-C	-8.34	88.48	111.00
2	B	240	GLU	N-CA-C	-7.18	91.61	111.00
2	D	12	ASP	N-CA-C	-7.13	91.75	111.00
3	K	173	LEU	CA-CB-CG	-7.12	98.91	115.30
2	H	321	TYR	N-CA-C	5.93	127.03	111.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4138	0	4080	177	0
1	C	4125	0	4065	181	0
1	E	4119	0	4054	201	0
1	G	4113	0	4058	171	0
2	B	3404	0	3385	202	0
2	D	3408	0	3396	176	0
2	F	3397	0	3380	234	0
2	H	3389	0	3359	238	0
3	I	668	0	702	36	0
3	J	604	0	638	37	0
3	K	604	0	638	40	0
3	L	604	0	638	53	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
4	H	1	0	0	0	0
All	All	32577	0	32393	1615	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

The worst 5 of 1615 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:143:LEU:HB3	3:J:150:MET:HE3	1.26	1.15
2:D:149:ILE:H	2:D:149:ILE:HD12	1.01	1.14
2:H:359:ALA:HB3	2:H:412:LEU:HD11	1.26	1.13
2:F:149:ILE:HD12	2:F:149:ILE:H	1.15	1.11
1:E:184:ARG:HH12	1:E:325:VAL:HG22	1.11	1.07

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	518/531 (98%)	451 (87%)	54 (10%)	13 (2%)	5	21
1	C	513/531 (97%)	452 (88%)	52 (10%)	9 (2%)	8	29
1	E	515/531 (97%)	464 (90%)	42 (8%)	9 (2%)	9	31
1	G	512/531 (96%)	447 (87%)	56 (11%)	9 (2%)	8	29
2	B	430/434 (99%)	376 (87%)	46 (11%)	8 (2%)	8	28
2	D	430/434 (99%)	370 (86%)	50 (12%)	10 (2%)	6	23
2	F	429/434 (99%)	360 (84%)	55 (13%)	14 (3%)	4	15
2	H	429/434 (99%)	355 (83%)	60 (14%)	14 (3%)	4	15
3	I	84/88 (96%)	78 (93%)	4 (5%)	2 (2%)	6	22
3	J	74/88 (84%)	70 (95%)	1 (1%)	3 (4%)	3	11
3	K	74/88 (84%)	65 (88%)	6 (8%)	3 (4%)	3	11
3	L	74/88 (84%)	65 (88%)	5 (7%)	4 (5%)	2	6
All	All	4082/4212 (97%)	3553 (87%)	431 (11%)	98 (2%)	6	22

5 of 98 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	252	LEU
1	C	252	LEU
2	D	116	PRO
2	D	204	LEU
1	E	202	ASP

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	452/462 (98%)	426 (94%)	26 (6%)	20	50
1	C	451/462 (98%)	424 (94%)	27 (6%)	19	49
1	E	448/462 (97%)	420 (94%)	28 (6%)	18	46
1	G	450/462 (97%)	429 (95%)	21 (5%)	26	59
2	B	378/382 (99%)	350 (93%)	28 (7%)	13	38
2	D	379/382 (99%)	354 (93%)	25 (7%)	16	44
2	F	377/382 (99%)	346 (92%)	31 (8%)	11	32
2	H	375/382 (98%)	351 (94%)	24 (6%)	17	45
3	I	73/74 (99%)	67 (92%)	6 (8%)	11	32
3	J	67/74 (90%)	62 (92%)	5 (8%)	13	37
3	K	67/74 (90%)	63 (94%)	4 (6%)	19	49
3	L	67/74 (90%)	66 (98%)	1 (2%)	65	87
All	All	3584/3672 (98%)	3358 (94%)	226 (6%)	18	46

5 of 226 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	J	171	LEU
2	H	348	GLN
1	E	517	ASN
2	H	321	TYR
1	G	516	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 145 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	343	GLN
2	H	439	HIS
1	G	436	HIS
2	H	262	GLN
1	C	447	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	522/531 (98%)	0.05	12 (2%) 60 58	33, 67, 99, 122	0
1	C	520/531 (97%)	0.07	5 (0%) 82 82	41, 68, 102, 130	0
1	E	521/531 (98%)	0.11	12 (2%) 60 58	32, 56, 116, 134	0
1	G	518/531 (97%)	0.14	18 (3%) 44 38	34, 64, 124, 137	0
2	B	432/434 (99%)	0.16	18 (4%) 36 32	36, 59, 109, 117	0
2	D	432/434 (99%)	0.27	17 (3%) 39 35	40, 70, 109, 117	0
2	F	431/434 (99%)	0.39	28 (6%) 18 14	37, 61, 116, 124	0
2	H	431/434 (99%)	0.29	26 (6%) 21 18	37, 69, 116, 122	0
3	I	86/88 (97%)	-0.05	0 100 100	47, 68, 93, 97	0
3	J	76/88 (86%)	0.34	3 (3%) 39 35	58, 77, 96, 98	0
3	K	76/88 (86%)	0.12	1 (1%) 77 77	56, 73, 90, 91	0
3	L	76/88 (86%)	0.53	5 (6%) 18 14	67, 93, 115, 121	0
All	All	4121/4212 (97%)	0.18	145 (3%) 44 38	32, 66, 113, 137	0

The worst 5 of 145 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	408	LEU	5.5
2	F	441	THR	5.3
2	H	360	LYS	5.2
1	C	259	PRO	5.1
1	G	201	LEU	5.0

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	ZN	F	4	1/1	0.97	0.18	62,62,62,62	0
4	ZN	D	3	1/1	0.99	0.19	74,74,74,74	0
4	ZN	B	1	1/1	0.99	0.16	65,65,65,65	0
4	ZN	H	2	1/1	0.99	0.17	80,80,80,80	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.